

Mean-Field vs Monte-Carlo equation of state for the expansion of a Fermi superfluid in the BCS-BEC crossover

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Abstract

The equation of state (EOS) of a Fermi superfluid is investigated in the BCS-BEC crossover at zero temperature. We discuss the EOS based on Monte-Carlo (MC) data and asymptotic expansions and the EOS derived from the extended BCS (EBCS) mean-field theory. Then we introduce a time-dependent density functional, based on the bulk EOS and Landau’s superfluid hydrodynamics with a von Weizsäcker-type correction, to study the free expansion of the Fermi superfluid. We calculate the aspect ratio and the released energy of the expanding Fermi cloud showing that MC EOS and EBCS EOS are both compatible with the available experimental data of ^6Li atoms. We find that the released energy satisfies an approximate analytical formula that is quite accurate in the BEC regime. For an anisotropic droplet, our numerical simulations show an initially faster reversal of anisotropy in the BCS regime, later suppressed by the BEC fluid.

I. INTRODUCTION

Current experiments with a Fermi gas of ^6Li or ^{40}K atoms in two hyperfine spin states operate in the regime of deep Fermi degeneracy. The experiments are concentrated across a Feshbach resonance, where the s-wave scattering length a_F of the interatomic Fermi-Fermi potential varies from large negative to large positive values. In this way it has been observed a crossover from a Bardeen-Cooper-Schrieffer (BCS) superfluid to a Bose-Einstein condensate (BEC) of molecular pairs [1–3].

The bulk energy per particle of a two-spin attractive Fermi gas can be expressed [1–5] in the BCS-BEC crossover by the following equation

$$\mathcal{E}(n) = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} f(y) , \quad (1)$$

where $k_F = (3\pi^2 n)^{1/3}$ is the Fermi wave vector, n is the number density, and $f(y)$ is a universal function of the inverse interaction parameter $y = (k_F a_F)^{-1}$, with a_F the Fermi-Fermi scattering length. The full behavior of the universal function $f(y)$ is unknown but one expects that in the BCS regime ($y \ll -1$) it has the following asymptotic behavior

$$f(y) = 1 + \frac{10}{9\pi y} + O\left(\frac{1}{y^2}\right) , \quad (2)$$

as found by Yang *et al.* [6,7] in 1957. In this regime the system is a Fermi gas of weakly bound Cooper pairs where the superfluid gap energy Δ is exponentially small. Instead, in the unitarity limit ($y = 0$) the energy per particle is proportional to that of a non-interacting Fermi gas and, from Monte-Carlo (MC) results [5], one finds

$$f(0) = 0.42 \pm 0.02 . \quad (3)$$

Finally, in the BEC regime ($y \gg 1$) the system is a weakly repulsive Bose gas of molecules of mass $m_M = 2m$, density $n_M = n/2$ and interacting with $a_M = 0.6a_F$ (from MC results [5] and 4-body theory [8]). In this BEC regime one expects the asymptotic expression

$$f(y) = \frac{5a_M}{18\pi a_F y} + O\left(\frac{1}{y^{5/2}}\right) , \quad (4)$$

as found by Lee, Yang and Huang [9], again in year 1957.

II. MONTE-CARLO VS MEAN-FIELD

We have recently shown [10] that the unknown universal function $f(y)$ can be modelled by the analytical formula

$$f(y) = \alpha_1 - \alpha_2 \arctan \left(\alpha_3 y \frac{\beta_1 + |y|}{\beta_2 + |y|} \right). \quad (5)$$

This formula has been obtained from Monte-Carlo (MC) simulations [5] and the asymptotic expressions. Table 1 of Ref. [10] reports the values of the interpolating value of α_1 , α_2 , α_3 , β_1 and β_2 . The thermodynamical formula

$$\mu(n) = \frac{\partial (n\mathcal{E}(n))}{\partial n} = \frac{\hbar^2 k_F^2}{2m} \left(f(y) - \frac{y}{5} f'(y) \right). \quad (6)$$

relates the bulk chemical potential μ to the energy per particle \mathcal{E} . We call Monte-Carlo equation of state (MC EOS) the equation of state $\mu = \mu(n, a_F)$ obtained from Eqs. (5) and (6).

Within the mean-field theory, the chemical potential μ and the gap energy Δ of the uniform Fermi gas are instead found by solving the following extended BCS (EBCS) equations [11,12]

$$-\frac{1}{a_F} = \frac{2(2m)^{1/2}}{\pi \hbar^3} \Delta^{1/2} \int_0^\infty dy y^2 \left(\frac{1}{y^2} - \frac{1}{\sqrt{(y^2 - \frac{\mu}{\Delta})^2 + 1}} \right), \quad (7)$$

$$n = \frac{N}{V} = \frac{(2m)^{3/2}}{2\pi^2 \hbar^3} \Delta^{3/2} \int_0^\infty dy y^2 \left(1 - \frac{(y^2 - \frac{\mu}{\Delta})}{\sqrt{(y^2 - \frac{\mu}{\Delta})^2 + 1}} \right). \quad (8)$$

By solving these two EBCS equations one obtains the chemical potential μ as a function of n and a_F . Note that EBCS theory does not predict the correct BEC limit: the molecules have scattering length $a_M = 2a_F$ instead of $a_M = 0.6a_F$. We call EBCS equation of state (EBCS EOS) the mean-field equation of state $\mu = \mu(n, a_F)$ obtained from Eqs. (7) and (8). Obviously, our MC EOS is much closer than the EBCS EOS to the MC results obtained in Ref. [5] with a fixed node technique.

For completeness, we observe that within the EBCS mean-field theory the condensate density n_0 of the Fermi superfluid can be written in terms of a simple formula [11,13], given by

$$n_0 = \frac{m^{3/2}}{8\pi\hbar^3} \Delta^{3/2} \sqrt{\frac{\mu}{\Delta} + \sqrt{1 + \frac{\mu^2}{\Delta^2}}}. \quad (9)$$

In Ref. [11] we have found that the condensate fraction is exponentially small in the BCS regime ($y \ll -1$) and goes to unity in the BEC regime ($y \gg 1$). A very recent MC calculation [14] has confirmed this behavior but find at the unitarity limit a condensate fraction slightly smaller ($n_0/(n/2) = 0.50$) than the mean-field expectation ($n_0/(n/2) = 0.66$).

III. TIME-DEPENDENT DENSITY FUNCTIONAL FOR A FERMI SUPERFLUID

We propose an action functional A which depends on the superfluid order parameter $\psi(\mathbf{r}, t)$ as follows

$$A = \int dt d^3\mathbf{r} \left\{ i\hbar \psi^* \partial_t \psi + \frac{c\hbar^2}{2m} \psi^* \nabla^2 \psi - U|\psi|^2 - \mathcal{E}(|\psi|^2)|\psi|^2 \right\}. \quad (10)$$

The term \mathcal{E} is the bulk energy per particle of the system, which is a function of the number density $n(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$. The Laplacian term $\frac{c\hbar^2}{2m} \psi^* \nabla^2 \psi$ accounts for corrections to the kinetic energy due to spatial variations. In the BCS regime, where the Fermi gas is weakly interacting, the Laplacian term is phenomenological and it is called *von Weizsäcker correction* [16]. In the BEC regime, where the gas of molecules is Bose condensed, the Laplacian term is due to the symmetry-breaking of the bosonic field operator and it is referred to as *quantum pressure*. Note that in the deep BEC regime our action functional reduces to the Gross-Pitaevskii action functional [15]. In our calculations we set the numerical coefficient c of the gradient term equal to unity ($c = 1$), to obtain the correct quantum-pressure term in the BEC regime. In the BCS regime, a better phenomenological choice for the parameter c could be $c = 1/3$ as suggested by Tosi *et al.* [17,18], or $c = 1/36$ as suggested by Zaremba and Tso [19].

For the initial confining trap, we consider an axially symmetric harmonic potential

$$U(\mathbf{r}, t) = \frac{m}{2} [\bar{\omega}_\rho(t)^2(x^2 + y^2) + \bar{\omega}_z(t)^2 z^2], \quad (11)$$

where $\bar{\omega}_j(t) = \omega_j \Theta(-t)$, with $j = 1, 2, 3 = \rho, \rho, z$ and $\Theta(t)$ the step function, so that, after the external trap is switched off at $t > 0$, the Fermi cloud performs a free expansion. The Euler-Lagrange equation for the superfluid order parameter $\psi(\mathbf{r}, t)$ is obtained by minimizing the action functional A . This leads to a time-dependent nonlinear Schrödinger equation (TDNLSE):

$$i\hbar \partial_t \psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + U + \mu(|\psi|^2) \right) \psi. \quad (12)$$

The nonlinear term μ is the bulk chemical potential of the system given by the MC EOS or the EBCS EOS. As noted previously, in the deep BEC regime this TDNLSE reduces to the familiar Gross-Pitaevskii equation. From the TDNLSE one deduces the Landau's hydrodynamics equations of superfluids at zero temperature by setting $\psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)} e^{iS(\mathbf{r}, t)}$, $\mathbf{v}(\mathbf{r}, t) = \frac{\hbar}{m} \nabla S(\mathbf{r}, t)$, and neglecting the term $(-\hbar^2 \nabla^2 \sqrt{n})/(2m\sqrt{n})$, which would vanish in the uniform regime. These hydrodynamics equations are

$$\partial_t n + \nabla \cdot (n \mathbf{v}) = 0, \quad (13)$$

$$m \partial_t \mathbf{v} + \nabla \left(\mu(n) + U(\mathbf{r}, t) + \frac{1}{2} m v^2 \right) = 0. \quad (14)$$

These superfluid equations differ from the hydrodynamic equations of a normal fluid in the superfluid velocity field being irrotational, i.e. $\nabla \wedge \mathbf{v} = 0$, so that the vorticity term $\mathbf{v} \wedge (\nabla \wedge \mathbf{v})$ does not appear in Eq. (14).

By using the superfluid hydrodynamics equations, the stationary state in the trap is given by the Thomas-Fermi profile $n_0(\mathbf{r}) = \mu^{-1} (\bar{\mu} - U(\mathbf{r}, 0))$. Here $\bar{\mu}$, the chemical potential of the inhomogeneous system, is fixed by the normalization condition $N = \int d^3\mathbf{r} n_0(\mathbf{r})$, where N is the number of Fermi atoms. By imposing that the hydrodynamics equations satisfy the scaling solutions for the density

$$n(\mathbf{r}, t) = n_0 \left(\frac{x}{b_1(t)}, \frac{y}{b_2(t)}, \frac{z}{b_3(t)} \right) / \prod_{k=1}^3 b_k(t), \quad (15)$$

and the velocity

$$\mathbf{v}(\mathbf{r}, t) = \left(x \frac{\dot{b}_1(t)}{b_1(t)}, y \frac{\dot{b}_2(t)}{b_2(t)}, z \frac{\dot{b}_3(t)}{b_3(t)} \right), \quad (16)$$

we obtain three differential equations for the scaling variables $b_j(t)$, with $j = 1, 2, 3 = \rho, \rho, z$. The dynamics is well approximated by evaluating the scaling differential equations at the center ($\mathbf{r} = \mathbf{0}$) of the cloud. In this case the variables $b_j(t)$ satisfy the local scaling equations (LSE)

$$\ddot{b}_j(t) + \bar{\omega}_j(t)^2 b_j(t) = \frac{\omega_j^2}{3 \prod_{k=1}^3 b_k(t)} \frac{\frac{\partial \mu}{\partial n}(\bar{n}(t))}{\frac{\partial \mu}{\partial n}(n_0(\mathbf{0}))}, \quad (17)$$

where $\bar{n}(t) = n_0(\mathbf{0}) / \prod_{k=1}^3 b_k(t)$. Clearly, the LSE depend critically on the EOS $\mu = \mu(n, a_F)$. The TDNLSE is solved by using a finite-difference Crank-Nicolson predictor-corrector method, that we developed to solve the time-dependent Gross-Pitaevskii equation [20]. Observe that imaginary-time integration of Eq. (12) by the Crank-Nicolson method generates the ground-state of Bose condensates in a ring and in a double-well [21] much more accurately than the steepest descent method used in the past. The simple LSE are instead solved by using a standardleap-frog symplectic algorithm, successfully applied to investigate the order-to-chaos transition in spatially homogeneous field theories [22].

In Ref. [23] we have compared our time-dependent theory with the available experimental data. Moreover, we have compared the full TDNLSE with the LSE by using both MC EOS and EBCS EOS. We have found that, using the same EOS, the TDNLSE gives results always very close to the LSE ones. Instead, we have found some differences between MC EOS and EBCS EOS. Figure 1 reports the aspect ratio and the released energy of a ^6Li cloud after 1.4 ms expansion from the trap realized at ENS-Paris [2]. In the experiment of Ref. [2] the free expansion of $7 \cdot 10^4$ cold ^6Li atoms has been studied for different values of $y = (k_F a_F)^{-1}$ around the Feshbach resonance ($y = 0$). Unfortunately, in this experiment the thermal component is not negligible and thus the comparison with the zero-temperature theory is not fully satisfactory. Figure 1 compares the experimental data of Ref. [2] with the LSE based on

both MC and EBCS equation of state. This figure shows that the aspect ratio predicted by the two zero-temperature theories exceeds the finite-temperature experimental results. This is not surprising because the thermal component tends to hide the hydrodynamic expansion of the superfluid. On the other hand, the released energy of the atomic gas is well described by the two zero-temperature theories, and the mean-field theory seems more accurate, also probably due to the thermal component. In Fig. 1 the released energy is defined as in Ref. [2], i.e. on the basis of the rms widths of the cloud. By energy conservation, the actual released energy is instead given by

$$E_{\text{rel}} = \int d^3\mathbf{r} \mathcal{E}[n_0(\mathbf{r})] n_0(\mathbf{r}) . \quad (18)$$

It is straightforward to obtain an analytical expression for the released energy assuming a power-law dependence $\mu = C n^\gamma$ for the chemical potential (polytropic equation of state) and writing $\mathcal{E}[n_0(\mathbf{r})] \simeq \frac{3}{5}\mu[n_0(\mathbf{r})] = \frac{3}{5}\frac{\bar{\mu}}{n_0(0)^\gamma}n_0(\mathbf{r})^\gamma$ where γ is the effective polytropic index, obtained as the logarithmic derivative of the chemical potential μ [10], namely

$$\gamma(y) = \frac{n}{\mu} \frac{\partial \mu}{\partial n} = \frac{\frac{2}{3}f(y) - \frac{2y}{5}f'(y) + \frac{y^2}{15}f''(y)}{f(y) - \frac{y}{5}f'(y)} . \quad (19)$$

In this way one finds the simple approximate formula

$$E_{\text{rel}} = \frac{3}{5}N\epsilon_F \frac{2(1 + \gamma(y))}{2 + 5\gamma(y)} f(y) , \quad (20)$$

where $\epsilon_F = \hbar^2 k_F(\mathbf{0})^2/(2m)$ is the Fermi chemical potential at the center of the trap, with $k_F(\mathbf{0}) = (3\pi^2 n_0(\mathbf{0}))^{1/3}$. Fig. 2 shows that this simple approximate formula which neglects all details of the initial aspect ratio produces fair semi-quantitative agreement, in particular in the BEC regime, with the actual released energy obtained by solving numerically Eq. (18).

During the free expansion of the cloud the aspect ratio in the BCS regime ($y \ll -1$) is measurably different from the one of the BEC regime ($y \gg 1$). In Ref. [23] we have predicted an interesting effect: starting with the same aspect ratio of the cloud, at small times ($t\omega_H \lesssim 3$) the aspect ratio is larger in the BCS region; at intermediate times ($t\omega_H \simeq 4$) the aspect ratio is enhanced close to the unitarity limit ($y = 0$); eventually at large times

($t\omega_H \gtrsim 5$) the aspect ratio becomes larger in the BEC region. Here $\omega_H = (\omega_\perp^2 \omega_z)^{1/3}$ is the geometric average of the trapping frequencies. This prediction is based on the numerical simulation of the LSE shown in Fig. 2, where we plot the aspect ratio of the expanding cloud as a function of the inverse interaction parameter $y = 1/(k_F a_F)$ at successive time intervals. At $t = 0$ the aspect ratio equals the trap anisotropy $\lambda = 0.34$. Of course the detailed sequence of deformations depends on the experimental conditions and in particular on the initial anisotropy, but the qualitative trend of an initially faster reversal on the BCS side, later suppressed by the BEC gas, is predicted for the expansion of any initially cigar-shaped interacting fermionic cloud.

IV. CONCLUSIONS

We have shown that the free expansion of a Fermi superfluid in the BCS-BEC crossover, that we simulate in a hydrodynamic scheme at zero temperature, reveals interesting features. We have found that the Monte-Carlo equation of state and the mean-field equation of state give similar results for the free expansion of a two-spin Fermi gas. The two theories are in reasonable agreement with the experimental data, which, however, are affected by the presence of a thermal component. Our Monte-Carlo equation of state and time-dependent density functional can be used to study many other interesting properties; for instance, the collective oscillations of the Fermi cloud [24,25,10], the Fermi-Bose mixtures across a Feshbach resonance of the Fermi-Fermi scattering length, and nonlinear effects like Bose-Fermi solitons and shock waves. Finally, we observe that new experimental data on collective oscillations [26] suggest that the Monte-Carlo equation of state is more reliable than the mean-field equation of state.

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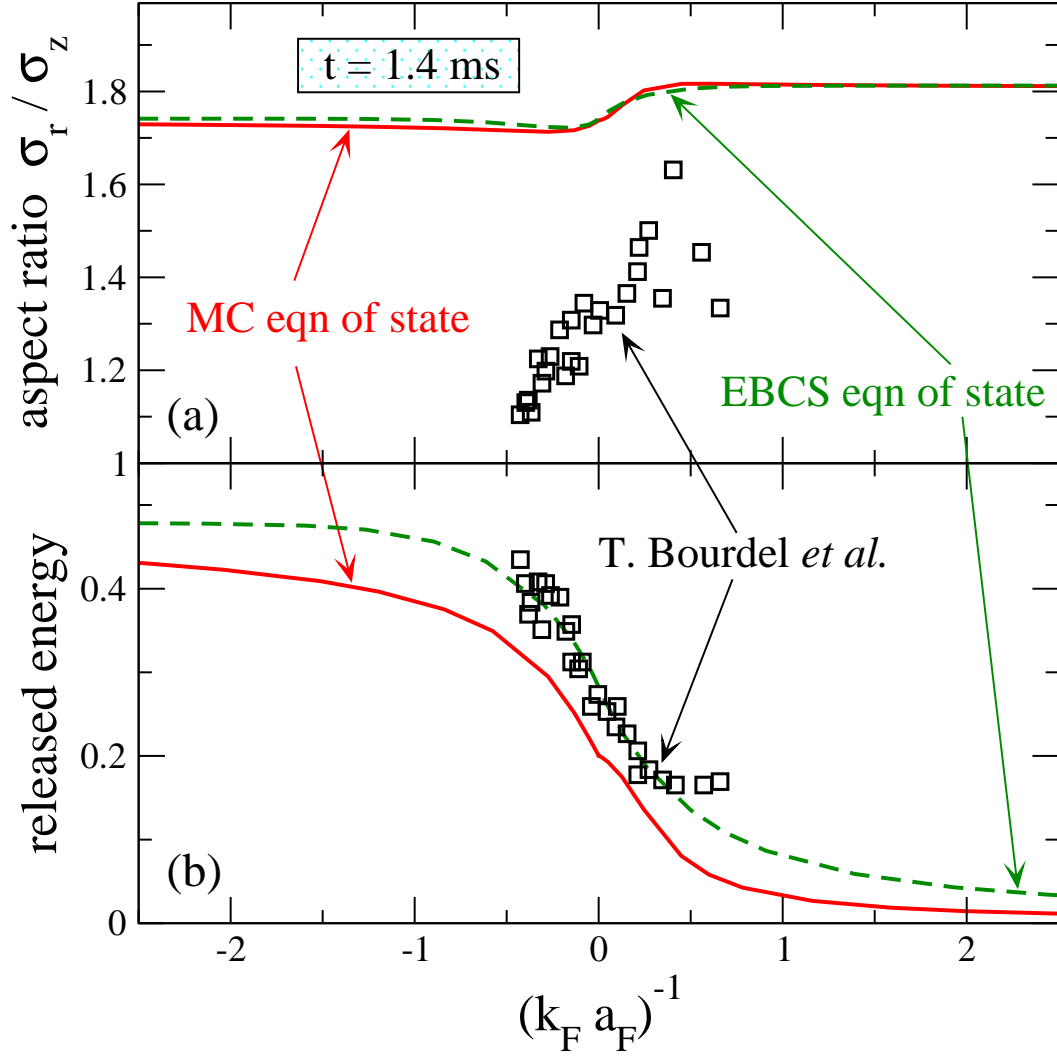


FIG. 1: Cloud of $N = 7 \cdot 10^4$ ${}^6\text{Li}$ atoms after 1.4 ms expansion from the trap realized at ENS-Paris [2] with anisotropy $\lambda = \omega_z/\omega_\rho = 0.34$. Squares: experimental data. Solid lines: numerical simulation with LSE and MC EOS; dashed lines: numerical simulation with LSE and EBCS EOS. The released energy is normalized as $E_{\text{rel}}/(N\epsilon_F)$.

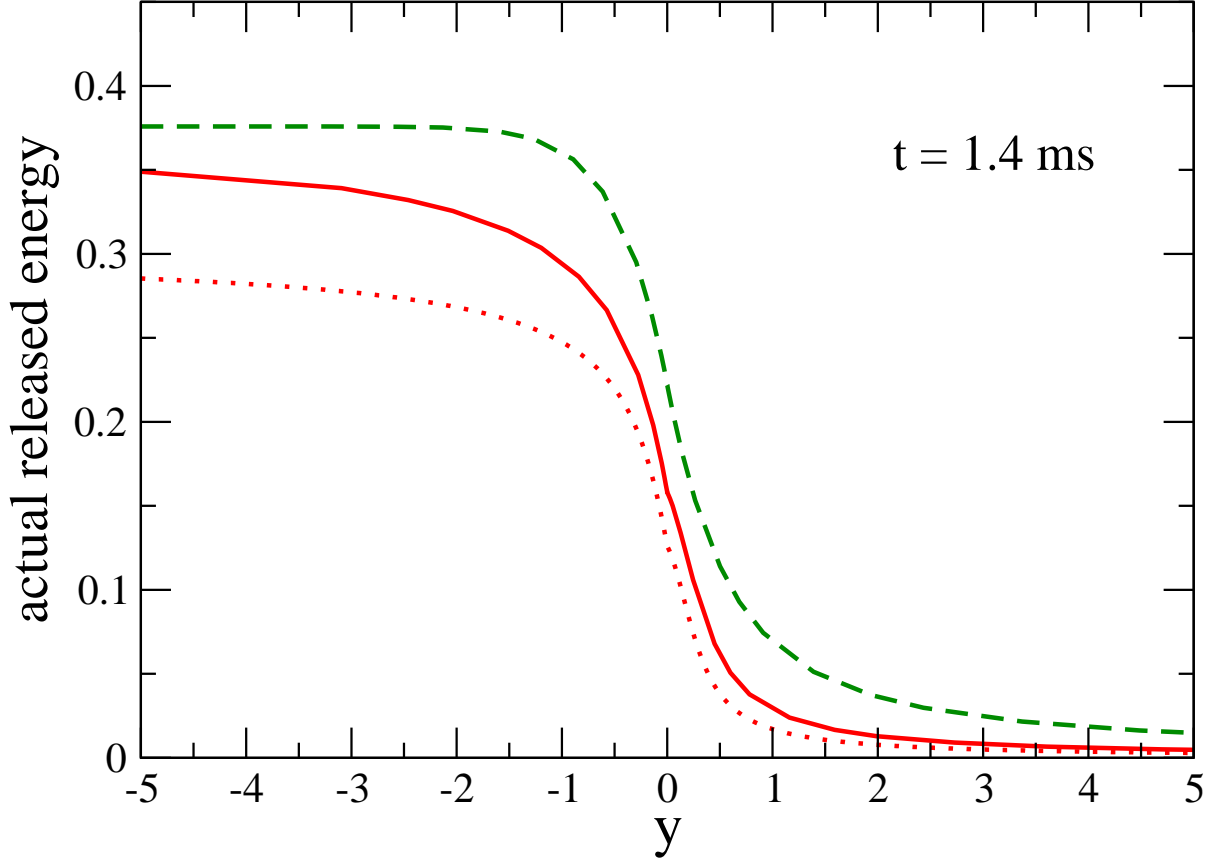


FIG. 2: Comparison of the approximate expression of Eq. (20) (dotted line) to the actual released energy defined in Eq. (18) for the conditions of the ENS-Paris experiment [2] (initial anisotropy $\lambda = \omega_z/\omega_\rho = 0.34$, $N = 7 \cdot 10^4$) (solid line). Both calculations assume the MC EOS. The actual released energy based on Eq. (18) and the EBCS EOS is also reported (dashed line).

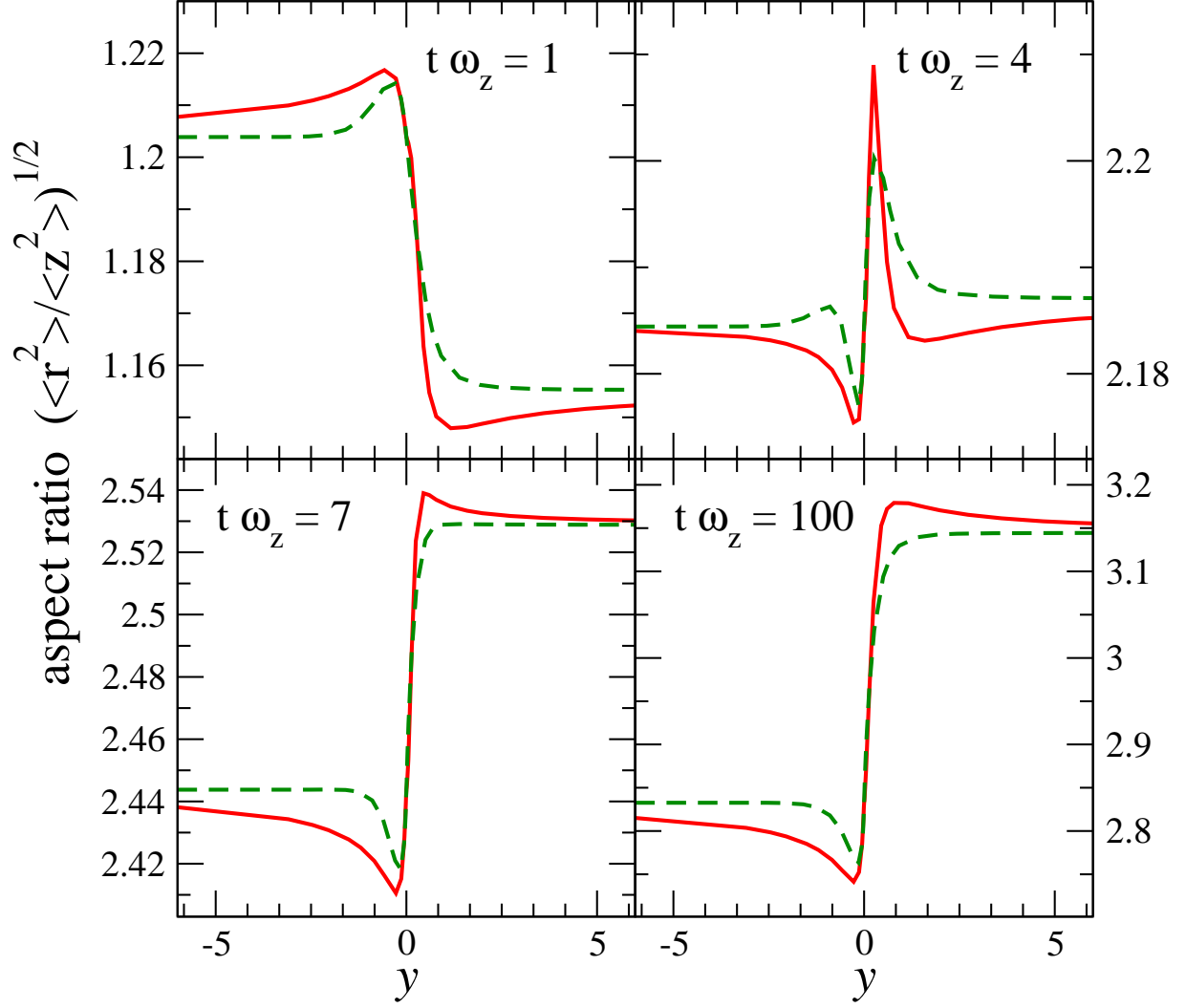


FIG. 3: Four successive frames of the aspect ratio of the ${}^6\text{Li}$ Fermi cloud as a function of $y = (k_F a_F)^{-1}$. At $t = 0$ the Fermi cloud is cigar-shaped with a constant aspect ratio equal to the initial trap anisotropy $\lambda = \omega_z/\omega_\rho = 0.34$. Solid lines: numerical simulation with LSE and MC EOS; dashed lines: numerical simulation with LSE and EBCS EOS.